

Anti-Alzheimer effects of the newly synthesized cationic compounds as multi-target dual hAChE/hBuChE inhibitor: An *in silico*, *in vitro*, and *in vivo* approach

Hosna Karami¹, Somaieh Soltani^{2*}, Gerhard Wolber³, Saeed Sadigh-Eteghad⁴, Roghaye Nikbakht⁵, Hanieh Farrokhi⁵, Farzaneh Narimani², Reza Teimuri-Mofrad⁵, Mohammad-Reza Rashidi^{2,6*}

¹Higher Education Institute of Rab-Rashid, Tabriz, Iran

²Pharmacy Faculty, Tabriz University of Medical Sciences, Tabriz, Iran

³Molecular Design Group, Pharmaceutical and Medicinal Chemistry, Institute of Pharmacy, Freie Universität Berlin, Germany

⁴Neurosciences Research Center, Tabriz University of Medical Sciences, Tabriz, Iran

⁵Department of Organic and Biochemistry, Faculty of Chemistry, University of Tabriz, 51666-16471, Tabriz, Iran

⁶Nanotechnology Research Center and Pharmacy Faculty, Tabriz University of Medical Sciences, Tabriz, Iran

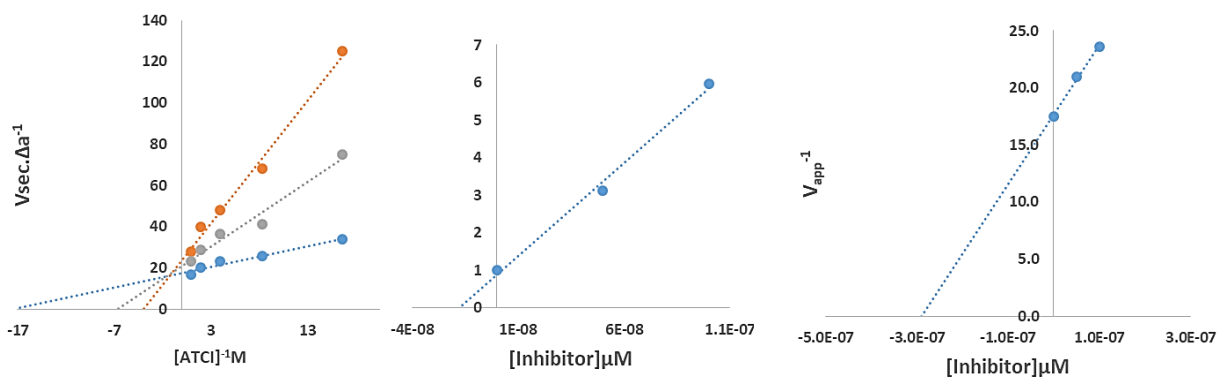


Fig. S2: Lineweaver–Burk and secondary plots of compound 5g

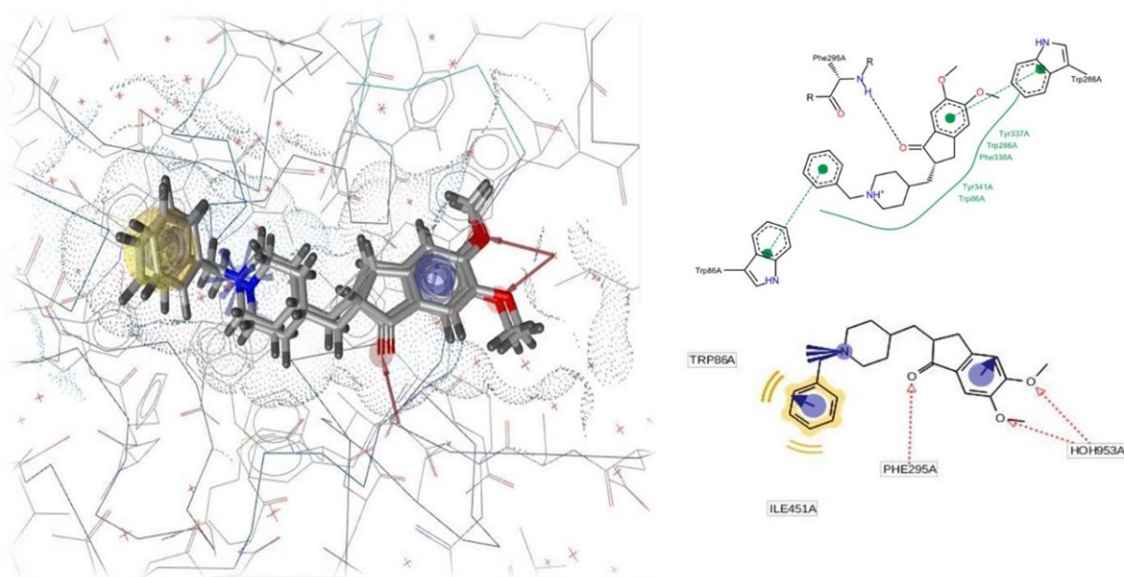


Fig. S3. 3D illustration of superimposition of docked Donpezil on cocrystallized donpezil (Pdb: 4EY7) (left) and cocrystallized butyrylthiocholine (Pdb: 1P0P) (right) along with pharmacophore mapping calculated by Ligandscout.